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# Calculations of the Energy and Angular Distribution of Electrons Ejected from Helium by Protons. II

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Doubly differential cross sections (ddcs), for ejection of secondary electrons of various energies and at various angles from helium bombarded by fast protons, have been calculated using the Born approximation. The wave functions of helium are approximated by products of one-electron orbitals. Results for the ddcs are given for several different choices of the one-electron orbitals, and these are compared with recent experimental values corresponding to 200- and 300-keV incident protons.

IN a previous paper[1] (referred to as I) calculations utilizing the Born approximation are given for the energy and angular distributions (doubly differential cross sections—ddcs) of electrons ejected from helium by high-energy protons. In these calculations, products of hydrogen-like wave functions are used throughout to approximate the wave functions of helium. At the time of I, experimental results were available for incident proton energies up to 150 keV.[2] Moderate agreement was found between the calculated and theoretical results with sizeable discrepancies in the forward and backward directions. Recently, experimental values of the ddcs have been obtained[3] at incident proton energies of 200 and 300 keV. The purposes of this paper are to give results of the calculations at higher incident energies and to give results for various choices of wave functions to represent helium in both its ground states and its continuum states.

In regard to the second purpose, the ddcs are calculated for the following three sets of wave functions: (1) the wave functions of I which are hydrogenlike except for a small modification to obtain orthogonality of the initial and final states; (2) the ground-state wave function is taken to be the four-term Roothaan[4] function and the continuum is hydrogenlike but modified to be orthogonal to the Roothaan ground state; and (3) same as the second set except that the $l=1$ part of the hydrogen-like continuum is replaced by a Hartree-Fock continuum.[5,6]

## THEORY

The ddcs $I$, differential in electron momentum $k$, and electron solid angle is given by

$$I=k^2\int|f_0^k|^2d\Omega, \tag{1}$$

where $d\Omega$ is the element of scattering for the proton.[1]

As in I, the wave functions for helium are approximated by products of single-electron wave functions. Let $\mathbf{r}_1$ and $\mathbf{r}_2$ be the position vectors of the two electrons. If atomic units are used and $\psi_k(\mathbf{r})$, the positive energy functions for the ejected particle are orthogonal to $\phi_0(r)$, the one-electron orbital for the ground state of helium; then[5]

$$f_0^k=C_1\int\psi_k^*(\mathbf{r}_1)\exp(i\mathbf{A}\cdot\mathbf{r}_1)\phi_0(r_1)\mathbf{dr}_1, \tag{2}$$

where

$$C_1=\frac{2\sqrt{2}\mu}{A^2}\int\phi_f^*(r_2)\phi_0(r_2)\mathbf{dr}_2.$$

Here $\mathbf{A}$ is the momentum-change vector in the center-of-mass system, $\phi_f$ is the wave function of the bound electron after ionization, and $\mu$ is the reduced mass of the two-body system.

[1] William J. B. Oldham, Jr., Phys. Rev. **140**, A1477 (1965).
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[3] M. E. Rudd, C. A. Sautter, and C. L. Bailey, Phys. Rev. **151**, 20 (1966).
[4] C. C. J. Roothaan, L. M. Sacks, and A. W. Weiss, Rev. Mod. Phys. **32**, 186 (1960).
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[6] A. L. Stewart and W. J. Wilkinson, Proc. Phys. Soc. (London) **75**, 796 (1960).

This paper, then, is concerned with using Eq. (2) to supply the integrand of Eq. (1) for the ddcs. The only choices left are the one-electron orbitals to be used for the initial and final states of the helium atom.

In the first calculation, the wave functions are those utilized in I. In a second calculation, $\phi_0$ in Eq. (2) is considered to be the Roothaan ground-state wave function,[4] i.e.,

$$\phi_0(r)=P_0(r)=N^{-1}(\beta_1 e^{-\alpha_1 r}+\beta_2 r e^{-\alpha_1 r}+\beta_3 e^{-\alpha_2 r}+\beta_4 r e^{-\alpha_2 r}), \tag{3}$$

with $\alpha_1=3.0$, $\alpha_2=1.4$, $\beta_1=0.429299$, $\beta_2=0.110917$, $\beta_3=1.47974$, $\beta_4=-0.169854$, and $N$ the normalization constant. The ejected particle, at large distances, moves in a Coulomb field of charge $z_3=1$. Hence, in the asymptotic region the ejected particle should be described by the hydrogen-like continuum wave function[5] $\phi_k(z_3\mid \mathbf{r})$ with $z_3=1$. However, $P_0(r)$ is not orthogonal to $\phi_k(z_3\mid \mathbf{r})$ if $z_3=1$ (or for any other $z_3$ for that matter). The simplest way to orthogonalize the pair is to modify the Coulomb continuum by subtracting off its projection onto the ground state, i.e.,

$$\psi_k(\mathbf{r})=\psi_k(1\mid \mathbf{r})-aP_0(r), \tag{4}$$

where $a=(1/N^2)\int\phi_k{}^{0*}(1\mid r)\,P_0(r)dr$ and $\phi_k{}^0$ is the $l=0$ part of $\phi_k$. ($a$ is real, so that $a^*=a$.)

In the third calculation, the ground-state wave function is the Roothaan four-term function, and the continuum wave function is a modification of Eq. (4):

$$\psi_k(\mathbf{r})=\phi_k(1\mid \mathbf{r})-\phi_k{}^{l=1}(1\mid \mathbf{r})+\phi_k{}^{l=1}(\text{H.F.}\mid \mathbf{r})-aP_0(r). \tag{5}$$

Here $\phi_k{}^{l=1}(1\mid \mathbf{r})$ is the $l=1$ part of the hydrogenlike continuum and $\phi_k{}^{l=1}(\text{H.F.}\mid \mathbf{r})$ is a Hartree-Fock–like continuum, the same as Stewart and Wilkinson[6] and Stewart and Webb[7] used in calculations of photoionization of helium.

For the first calculation, the Born matrix element and the indicated integrations over $\mathbf{dr}_1$ are given in I. The results for I can be written as follows:

$$I=C_0{}^2k^2\int\mid W_1-W_2(1)+W_2(1.6875)\mid{}^2d\Omega, \tag{6}$$

with

$$C_0=\frac{2^{3/2}\mu z_1{}^3}{\pi A^2}\int\phi_0{}^*(z_3\mid r)\,e^{-z_1 r}\mathbf{dr},$$

and

$$z_2=2,$$

and where

$$W_1=\int\phi_k{}^*(z_3\mid \mathbf{r})\,\exp(i\mathbf{A}\cdot\mathbf{r})\,e^{-z_1 r}\mathbf{dr},$$

with

$$W_2=\int\phi_k{}^{0*}(z_3\mid r)\,\exp(i\mathbf{A}\cdot\mathbf{r})e^{-z_1 r}\mathbf{dr}.$$

The results of performing the integrations over $\mathbf{dr}$ for $W_1$ and $W_2$ are given in the Appendix.

The wave functions of Eqs. (3) and (4) are now used in Eq. (2) for the Born matrix element. The matrix element is now written as

$$f_0{}^k=C_R\left[\int\phi_k{}^*(1\mid \mathbf{r})\,\exp(i\mathbf{A}\cdot\mathbf{r})\,P_0(r)\mathbf{dr}-a\int P_0{}^2(r)\,\exp(i\mathbf{A}\cdot\mathbf{r})\mathbf{dr}\right], \tag{7}$$

where

$$C_R=\frac{8\mu}{(\sqrt{\pi})A^2N^2}\int e^{-2r_2}P_0(r_2)\,\mathbf{dr}_2.$$

Since $P_0(r)$ is the sum of four terms, the first term of the Born matrix element in Eq. (7) can be written as the sum of four integrals. From observation of the form $P_0(r)$, the first term of $f_0{}^k$, $f_{0\mathrm{I}}{}^k$ can be written in terms of $W_1$ and $\partial W_1/\partial Z_1$ (cf. Appendix):

$$f_{0\mathrm{I}}{}^k=\frac{4\mu C_R}{A^2}\left[\beta_1 W_1(3,1)-\beta_2\frac{\partial W}{\partial Z_1}(3,1)+\beta_3 W_1(1.4,1)-\beta_4\frac{\partial W_1}{\partial Z_1}(1.4,1)\right]. \tag{8}$$

Here, $W_1(Z_1, Z_3)$ refers to $W_1$ considered as a function of the parameters $Z_1$ and $Z_3$. In the first two terms of Eq. (8) $Z_1=\alpha_1$, and in the second two terms $Z_2=\alpha_2$. Hence, most of the integration for $f_{0\mathrm{I}}{}^k$ has already been carried out. Calculating the derivative of $W_1$ with respect to $Z_1$ is tedious, but straightforward. The result is given in the Appendix.

The second term of Eq. (7), $f_{0\mathrm{II}}{}^k$, can be evaluated easily, and the result is

$$\begin{aligned}f_{0\mathrm{II}}{}^k=4\pi C_R[&4\alpha_1\beta_1{}^2/A_1{}^2+48\alpha_1\beta_1{}^2(4\alpha_1{}^2-A^2)/A_1{}^4\\&+4\beta_3{}^2\alpha^2/A_2{}^2+48\alpha_2\beta_4(4\alpha_2{}^2-A^2)/A_2{}^4\\&+4\beta_1\beta_2(12\alpha_1{}^2-A^2)/A_1{}^3+4\beta_1\beta_2(\alpha_1+\alpha_2)/A_{12}{}^2\\&+(4/A_{12}{}^3)[3(\alpha_1+\alpha_2)^2-A^2](\beta_1\beta_4+\beta_2\beta_3)\\&+48\beta_2\beta_4(\alpha_1+\alpha_2)[(\alpha_1+\alpha_2)^2-A^2]/A_{12}{}^4\\&+2\beta_3\beta_4(12\alpha_2{}^2-A^2)/A_2{}^3],\end{aligned} \tag{9}$$

where $A_1=A^2+4\alpha_1{}^2$, $A_2=A^2+4\alpha_2{}^2$, and $A_{12}=A^2+(\alpha_1+\alpha_2)^2$.

The result for $a$ of Eq. (7) can be found from Eq. (9) if $C_R$ is omitted and $A=0$. Then the Born matrix element is given by $f_0{}^k=f_{0\mathrm{I}}{}^k+f_{0\mathrm{II}}{}^k$.

[7] A. L. Stewart and T. G. Webb, Proc. Phys. Soc. (London) **82**, 532 (1963).

With the wave functions of Eqs. (3) and (5), the Born matrix element becomes

$$f_0^k = C_R\Big[\int \phi_k^*(1\mid \mathbf{r})\,\exp(i\mathbf{A}\cdot\mathbf{r})\,P_0(r)\,d\mathbf{r} + \int \phi_k^{l=1}(\text{H.F.}\mid \mathbf{r})\,\exp(i\mathbf{A}\cdot\mathbf{r})\,P_0(r)\,d\mathbf{r} - \int \phi_k^{l=1}(1\mid \mathbf{r})\,\exp(i\mathbf{A}\cdot\mathbf{r})\,P_0(r)\,d\mathbf{r} - a\int P_0^2(r)\,\exp(i\mathbf{A}\cdot\mathbf{r})\,d\mathbf{r}\Big]. \quad (10)$$

Everything in Eq. (10) has been evaluated except the second and third terms. The third term, which involves the $l=1$ part of the hydrogen continuum, can be evaluated analytically. However, since the $l=1$ part of the hydrogen wave must be calculated numerically to compute the relative phase shift of the Hartree-Fock wave, it is easier to calculate the difference of the second and third terms numerically. If $I_F$ and $I_W$ are the second and third terms of Eq. (10), respectively, then

$$I_F - I_W = -\frac{6e^{i\sigma_c}}{k(2\pi)^{1/2}A^2}\cos\theta\int_0^\infty \frac{P_0(r)}{r} \times[\sin Ar - Ar\cos Ar][f_l(kr)\,e^{i\sigma_1} - g_l(kr)]\,dr,$$

where $f_l(kr)$ is the Hartree-Fock wave and $g_l(kr)$ is the Coulomb wave. $\sigma_c$ is the phase of the Coulomb wave; $\sigma_1$ is the phase of the Hartree-Fock wave with respect to the Coulomb wave; $\theta$ is the angle between $\mathbf{A}$ and $\mathbf{k}$.

In each case, it is necessary to perform the double integration over $d\Omega$ for $I$ of Eq. (1). To accomplish this, the reference direction must be changed to a fixed direction in space. In this case, it is convenient to use the incident-proton direction as a reference direction. Suppose the electron is ejected in the direction $(\chi, 0)$ and the proton is scattered in the direction $(\delta, \rho)$, as shown in Fig. 1. The expressions for $A$ and $\cos\theta$ are given in I.

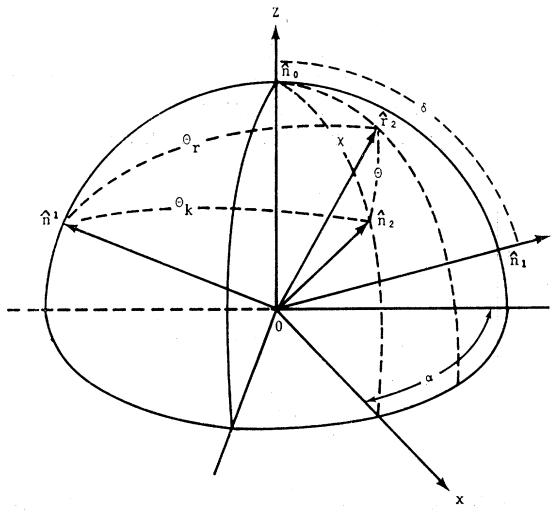


FIG. 1. Directions of the incident and scattered particles. $\hat{n}_0$, direction of incidence; $\hat{n}_1$, direction of scattering; $\hat{n}_2$, direction of ejection; $\hat{n}^1$, direction of change of momentum of incident proton.

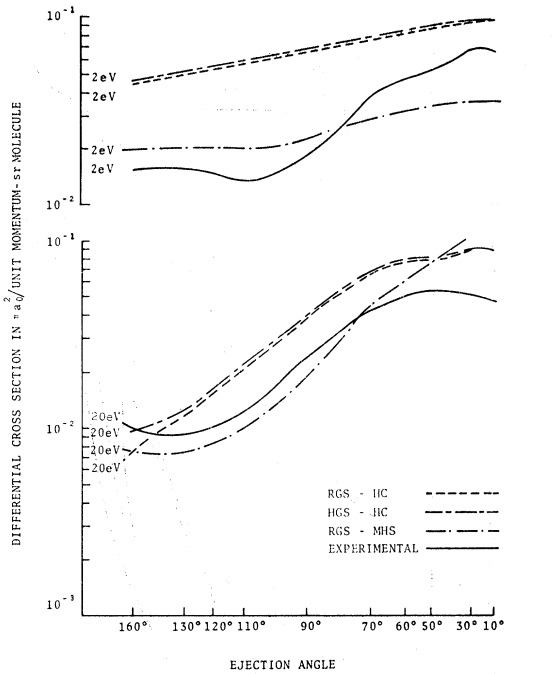


FIG. 2. Differential cross section for production of secondary electrons by 200-keV protons in helium. RGS–HC: Results of using the Roothaan ground-state wave function and the hydrogenlike continuum. HGS–HC: Results of using the hydrogenlike ground-state wave function and the hydrogenlike continuum. RGS–MHC: Results of using the Roothaan ground-state wave function and the hydrogenlike continuum modified by the $l=1$ part replaced by the Hartee-Fock continuum.

The double integration indicated in Eq. (1) can now be carried out over $\delta$ and $\rho$. A computer program was written to perform these integrations for input parameters of $E_0$, $E_j$, and $\chi$. Samples of results of these calculations are presented in Figs. 2–5, which also show the experimental results for comparison. In addition to results for calculations for the three calculations given above, the results using the Roothaan ground state and the hydrogen-like continuum without the orthogonalization correction are also presented. At the higher ejection energies, the overlap integral is negligible and the correction does not make any changes in the cross section. In the case of calculation III, the change of the $l=1$ part of the continuum wave function from hydrogen-like to Hartree-Fock makes no perceptible change in the ddcs.

## DISCUSSION OF RESULTS

The figures show that if the orthogonal correction term of Eq. (4) is neglected, the cross sections are al-

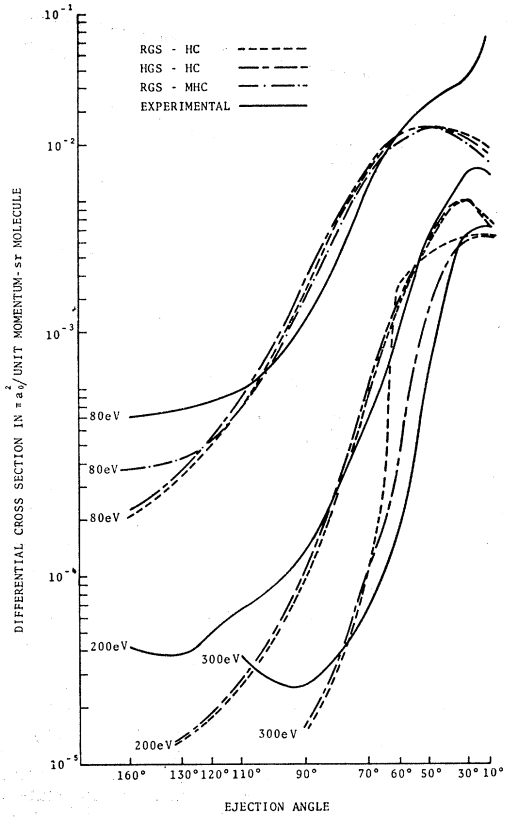


FIG. 3. Differential cross section for production of secondary electrons by 200-keV protons in helium.

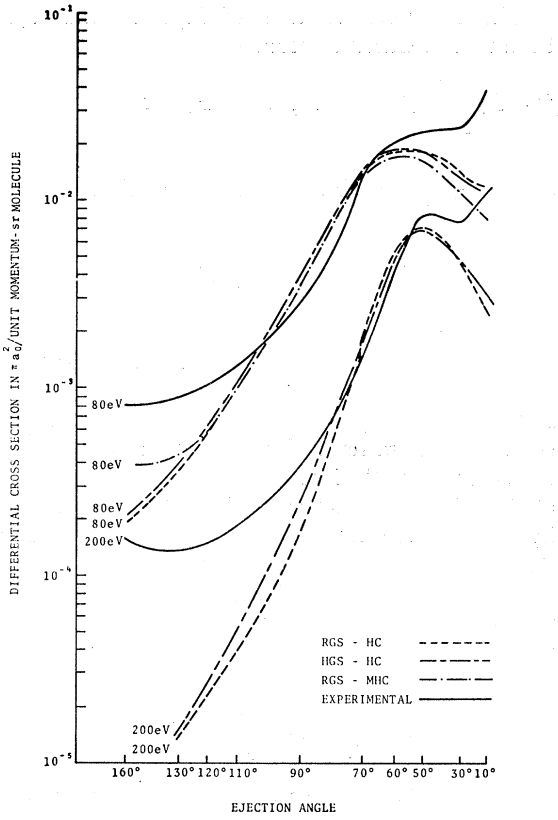


FIG. 5. Differential cross section for production of secondary electrons by 300-keV protons in helium.

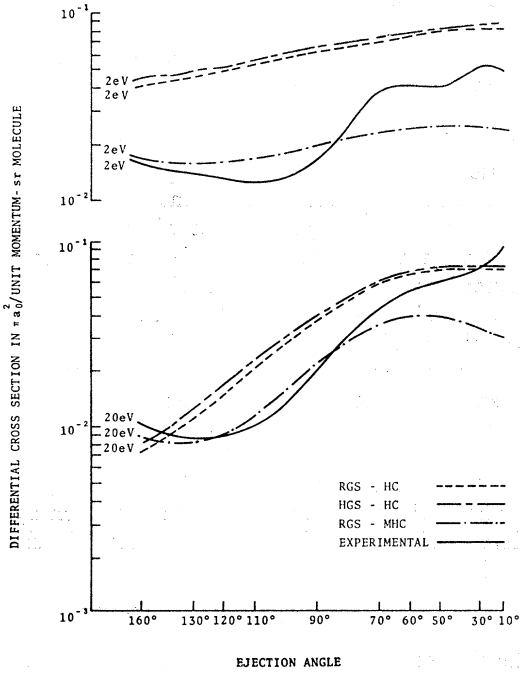


FIG. 4. Differential cross section for production of secondary electrons by 300-keV protons in helium.

most identical to those for the hydrogenlike ground state. When the correction for nonorthogonality is considered, it appears that there is an over-all improvement in the cross sections, although the result at any one ejection angle and ejection energy may not improve, particularly at the low-ejection energies. Although the calculation with the continuum orthogonalized with respect to the Roothaan ground state yields results in better agreement with experiment over a wider range of angles than the calculation with the

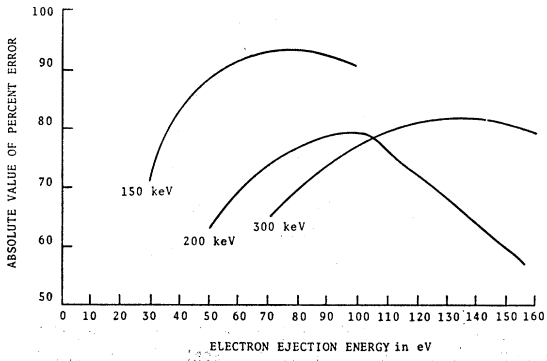


FIG. 6. Absolute error in the differential cross section versus electron ejection energy.

hydrogenlike ground state or the nonorthogonal Roothaan ground state, there is no guarantee that the Roothaan ground state is appropriate for these calculations. The Roothaan function is a fit to the Hartree-Fock ground state which is found from the minimum principle of energy. The matrix elements involved in the ddcs emphasize a different region of configuration space than does the energy matrix element.

Certainly the method used here is not the only one that can be used to gain orthogonality between the Roothaan ground state and the hydrogen-like continuum. It is merely the simplest and the easiest. However, the $l=0$ part of the resultant continuum-wave function probably does not represent the $s$-wave very accurately. The correction for nonorthogonality is largest at low ejection energies, which contribute most heavily to the total cross section. Hence, if total cross sections are desired, it seems clear that orthogonalized wave functions should be used.

The change of the $l=1$ wave function from the hydrogen-like to the Hartree-Fock makes very little change in the ddcs. Since Stewart and Webb found good agreement for photo-ionization of helium using this wave function, one might expect an improvement in the ddcs. In these calculations no such improvements have been found.

One can speculate why such "improvements" do not make corresponding changes in the ddcs. Suppose for a moment that the reason for the discrepancy in the forward direction is due to an interaction between the scattered proton and the ejected electron. If this were so, one would think that this interaction would be the greatest when the relative velocity of the proton and electron is the smallest. This should reflect into the ddcs. In fact, the theoretical error of the ddcs should be the greatest when the ejected electron and scattered proton have the same speed. Figure 6 shows plots of the relative error $E=|(I_{\text{expt}}-I_{\text{th}})/I_{\text{expt}}|\times 100$ versus ejected energy for the cases of 150, 200, and 300 keV at ejection angle of 10°. In each of the above cases, the maximum of the curve appears where the velocities of the two particles are equal. This picture seems to indicate that a strong interaction between the ejected electron and scattered proton causes the enhanced ejection in the forward direction. However, an "interaction between the ejected electron and the scattered proton" is evidence of possible failure of the Born approximation, since the corresponding Coulomb interaction is in the Born matrix element. Or perhaps this is a consequence of the inadequacy of the wave functions, since we are asking for great detail in a small angular range. The wave functions could be inadequate for those parts of configuration space that contribute most heavily to the cross section in that angular region.

## CONCLUSIONS

Although some improvement can be made in the over-all ddcs by using a more complicated ground-state wave function, such as the four-term Roothaan ground state, new problems appear when this method is used. For example, a continuum-state wave function must be constructed that satisfies the orthogonality conditions.

Further, the results still leave unsolved discrepancies in the forward and back directions. For instance, the theory always predicts an absolute maximum at some $0°<\theta<90°$, depending on the ejection energy. The experiment sometimes show a local maximum here but has an absolute maximum in the forward direction. The cause of this discrepancy is not clear; however, it is probably not due to either inaccuracy in the wave functions or inherent errors in the Born approximation.

## APPENDIX

The expressions for $W_1$, $W_2$, and $\partial W_1/\partial Z_1$ are as follows:

$$W_1=-4\left[\frac{Z_3/k}{1-\exp(-i2\pi Z_3/k)}\right]^{1/2}\frac{f+ig}{S^2R^{1/2}}\exp\left[\frac{-Z_3}{k}E+i\left(\frac{Z_3}{k}L+E\right)\right],$$

$$W_2=-\frac{2}{A}\left[\frac{Z_3/k}{1-\exp(-2\pi Z_3/k)}\right]^{1/2}\frac{[(A^2-Z_1^2-k^2)\sin\nu+2Z_1A\cos\nu]}{[(k+A)^2+Z_1^2][(k-A)^2+Z_1^2]}\exp(-Z_3E/k),$$

where

$$f=(k^2-Z_1^2)(Z_1-Z_3)-A^2(Z_1+Z_3)+2Z_3AK\cos\theta,$$

$$g=2Z_1[k(Z_1-Z_3)+Z_3A\cos\theta],$$

$$E=\tfrac{1}{2}\pi-\tan^{-1}[(A^2-k^2+Z_1^2)/2kZ_1],$$

$$L=\ln\frac{k^2+A^2+Z_1^2-2Ak\cos\theta}{[(A^2-k^2+Z_1^2)+4k^2Z_1^2]^{1/2}},$$

$$S=k^2+A^2+Z_1^2-2Ak\cos\theta,$$

$$R=(A^2-k^2+Z_1^2)^2+4k^2Z_1^2,$$

$$\nu=\frac{Z_3}{2k}\ln\left[\frac{(k+A)^2+Z_1^2}{(k-A)^2+Z_1^2}\right],$$

and $\theta$ is the angle between **A** and **k**.

If

$$C_w=-4\left[\frac{Z_3/k}{1-\exp(-2\pi Z_3/k)}\right]^{1/2},$$

one gets

$$\frac{\partial W_1}{\partial Z_1}=W\left[i\frac{Z_3}{k}\frac{\partial L(Z_1)}{\partial Z_1}+\left(i-\frac{Z_3}{k}\right)\frac{\partial E(Z_1)}{\partial Z_1}\right]+\frac{C_w\exp[-Z_3E(Z_1)/k]}{S^3(Z_1)R^{3/2}(Z_1)}$$
$$\times\exp\{i[(Z_3/k)L(Z_1)+E(Z_1)]\}\{S(Z_1)R(Z_1)[\partial f(Z_1)/\partial Z_1+i\partial g(Z_1)/\partial Z_1]-G(Z_1)\},$$

with

$$G(Z_1)=[f(Z_1)+ig(Z_1)]\{4Z_1R(Z_1)+\tfrac{1}{2}[S(Z_1)]\partial R(Z_1)/\partial Z_1\}.$$

The noted derivatives are as follows:

$$\partial f(Z_1)/\partial Z_1=k^2-A^2-3Z_1^2+2Z_1Z_3,$$
$$\partial g(Z_1)/\partial Z_1=g(Z_1)/Z_1+2kZ_1,$$
$$\partial L(Z_1)/\partial Z_1=2Z_1/R(Z_1)S(Z_1)[R(Z_1)-(A^2+Z_1^2+k^2)S(Z_1)],$$
$$\partial S(Z_1)/\partial Z_1=2Z_1,$$
$$\partial E(Z_1)/\partial Z_1=-2k(Z_1^2-A^2+k^2)/R(Z_1),$$
$$\partial R(Z_1)/\partial Z_1=4Z_1(A^2+Z_1^2+k^2).$$

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# Lamb Shift in the $(Li^6)^{++}$ Ion*

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The energy difference between the $2S_{1/2}$ and $2P_{1/2}$ levels of the hydrogen-like atom $(Li^6)^{++}$ was determined by measuring the lifetime of the metastable $2S_{1/2}$ state in an electrostatic field (Stark quenching). The metastable ions were produced by charge equilibrating a lithium beam of energy ~3 MeV in nitrogen gas and were then directed through the electrostatic field (about 10 kV/cm) between a pair of parallel plates. The field mixed the $2S_{1/2}$, $2P_{1/2}$, and $2P_{3/2}$ states and the photons from the subsequent decay from $2P$ to the ground state were detected with two thin-window GM counters, one of them fixed and the other movable along the quenching chamber in the beam direction. From the normalized counting rates of the movable counter and the separation between the two counters, the lifetime of the perturbed $2S$ state could be determined. It was found to be $(2.629\pm0.021)\times10^{-9}$ sec and $(1.764\pm0.035)\times10^{-9}$ sec for the field strengths $7425\pm2$ and $9173\pm2$ V/cm, respectively. From these values, the Bethe-Lamb theory of Stark quenching yields an averaged Lamb shift in the $(Li^6)^{++}$ ion of $63\,031\pm327$ Mc/sec. This result agrees with the theoretical value $62\,740\pm47$ Mc/sec recently calculated by Erickson.

## I. INTRODUCTION

In a series of high-precision experiments using microwave techniques, the energy difference between the $2S_{1/2}$ and $2P_{1/2}$ level of a hydrogen atom was established by Lamb and his collaborators at $1057.77\pm0.10$ Mc/sec.[1–6] The corresponding shift in a $He^+$ ion was also measured precisely as $14\,040.2\pm4.5$ Mc/sec.[7,8] These deviations from the prediction of the Dirac

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